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**ION AND ELECTRON DISTRIBUTIONS
IN THE BOUNDARY LAYER OF HYPERSONIC
VEHICLES FOR CHEMICAL NONEQUILIBRIUM FLOW**

**Part II
METHOD OF SOLUTION AND COMPUTER PROGRAM**

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ABSTRACT

Various computational aspects have been investigated to numerically solve charge-conservation equations and Poisson's equation for the electric field yielding ion and electron distributions. These equations were derived and presented by the Harry Diamond Laboratories as part I of this study. The computational aspects, reported herein as part II of the study, include: (1) transformations to reduce the steep slopes of the input functions and to simplify the solutions of the equations; (2) linearization of the equations to permit use of matrix methods in their solution; (3) derivation of small-value, asymptotic solutions to provide starting conditions in the matrix solution; (4) a computer program listing, description, and sample output; and (5) descriptions of an independent check solution and other checks to confirm validity of the results. The computer program is written to accommodate any consistent set of boundary conditions. Although the equations are linearized, the nonlinear terms are approximated in a way to insure rapid convergence of solutions to the exact equations.

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A study has been conducted by the Harry Diamond Laboratories of ion-electron distributions for a hypersonic vehicle with a 10-degree semivertex, sharply pointed cone at Mach 8 and 10 for sea-level flight. Detailed calculations are reported by Pollin¹ as part I of this study. This report, which represents part II of the study, is concerned specifically with computational aspects of the ion-electron-distribution equations detailed in part I.¹ The equations to be solved are presented herein to describe the transformations required to simplify their numerical solution. Readers who are particularly interested in the derivation and precise symbol definitions should refer to part I.¹

Basically, a parabolic system of five first-order, partial differential equations describe the phenomenon (listed as equations 18 and 20 in part I). Use of the compact " \pm " notation to condense two equations into one is shown below.

$$\frac{\pm J}{en_e} = -\frac{\pm}{s} \left[\frac{v(x,y)}{P(\eta)} \right]_{\eta} - \frac{W(\eta, \bar{s}, \bar{s})}{\rho_e c_e} \delta(x) + \frac{u(\eta) \delta(x)}{P(\eta)} \frac{\pm}{s} x \quad (1)$$

$$\frac{\pm}{s} \eta = \frac{\delta(x) P(\eta) \frac{\pm J}{en_e} + \delta(x) v(x,y) \frac{\pm}{s} \mp \bar{K}(\eta) \frac{\pm}{s} \phi_{\eta}}{\frac{\pm}{s} D(\eta) + D_T(x, \eta)} \quad (2)$$

$$\phi_{\eta\eta} = -\frac{10^{14}}{8.95} en_e \frac{[\delta(x)]^2}{P(\eta)} (\frac{\pm}{s} - \bar{s}) \quad (3)$$

Equations (1) and (2) are each two equations--read first with upper and then with lower signs whenever two signs appear. The dependent variables are J , \bar{J} , s , \bar{s} , and ϕ ; the independent variables are $0 \leq x \leq \infty$ and $0 \leq y \leq \delta(x)$ with η defined by

$$\eta = \frac{y}{\delta(x)} \quad (4)$$

so that $0 \leq \eta \leq 1$ is used as a normalized independent variable. This is convenient also because many of the input functions are ultimately functions of η . The other symbols are either constants (ρ_e , c_e , e , n_e), or other known functions [$P(\eta)$, $v(x,y)$, $W(\eta, \bar{s}, \bar{s})$, $\delta(x)$, $u(\eta)$, $D(\eta)$, $D_T(x, \eta)$, $\bar{K}(\eta)$]; some of the constants and functions change with geometry, velocity, and altitude of the vehicle.

¹Pollin, I., "Ion and Electron Distributions in the Boundary Layer of Hypersonic Vehicles for Chemical Nonequilibrium Flow--Part I: Aerodynamics and Numerical Results," HDL-TR-1565, August 1971.

Subscripts x and η indicate partial derivatives with respect to these variables. Note that ϕ does not appear except with subscript η ; ϕ_η is considered as a basic dependent variable. The voltage ϕ is calculated once ϕ_η is obtained.

The known functions are sometimes derived from formulas and sometimes are calculated in point-data form. We have

$$\delta(x) = bx^{0.8}, \quad b \text{ constant}, \quad (5)$$

$$u(\eta) = u_\delta \eta^{1/8}, \quad u_\delta \text{ constant}, \quad (6)$$

$$W(\eta, \bar{s}, \bar{s}) = KFNO(\eta) - B(\eta) \bar{s} \bar{s} \quad (7)$$

where $KFNO$ is used for $K_f \langle N \rangle \langle 0 \rangle$ and $B(\eta)$ is used for $K_r [n_e / P(\eta)]^2$. Both K_f and K_r are found as functions of the known temperature function $T \equiv T(\eta)$:

$$K_f = \frac{5 \times 10^{-11} \exp(-32,500/T)}{T^{0.5}} \quad (8)$$

$$K_r = 3 \times 10^{-3} / T^{1.5}$$

Also,

$$\bar{K}(\eta) = \frac{11,600}{T(\eta)} D(T) \quad (9)$$

$$D_T(x, \eta) = 0.02 u_\delta \delta(x) \eta^{9/8} \quad (10)$$

and $\bar{D}(T)$ and $\bar{D}(T)$ are related by

$$\bar{D}(T) = 234 \bar{D}(T) \quad (11)$$

Finally, $v(x, y)$ must satisfy

$$\left[u_\delta \frac{x}{P(\eta)} \eta^{1/8} \right]_x + x \left[\frac{v(x, y)}{P(\eta)} \right]_y = 0 \quad (12)$$

with $v(x, 0) = 0$. A lengthy computation shows that in the case considered here,

$$v(x, y) = u_\delta \frac{\delta(x)}{x} f(\eta) \quad (13)$$

where $f(\eta)$ is given by

$$f(\eta) = 0.8 \eta^{9/8} - P(\eta) \int_0^\eta \frac{1.8 t^{1.8}}{P(t)} dt \quad (14)$$

System (1) to (3) is also subject to boundary conditions; if $\bar{s}(x, \eta)$, $\bar{J}(x, \eta)$, and $\phi_\eta(x, \eta)$ are solutions, we have

$$\bar{s}^+(0, \eta) = \bar{s}^-(0, \eta) = 0 \quad (15)$$

$$\bar{s}^+(x, 0) = \bar{s}^-(x, 0) = 0 \quad (16)$$

$$\bar{s}^+(x, 1) = \bar{s}^-(x, 1) = \phi_\eta(x, 1) = 0 \quad (17)$$

2. THE J' TRANSFORMATION

A convenient simplification to system (1) to (3) results from transformation of the current variables \bar{J} to \bar{J}' defined by

$$\bar{J}' = \left[\frac{\bar{J}}{en_e} + \frac{\bar{s}v(x, y)}{P(\eta)} \right] \delta(x) \quad (18)$$

By taking a derivative with respect to η ,

$$(\bar{J}')_\eta = \left[\left(\frac{\bar{J}}{en_e} \right)_\eta + \bar{s}_\eta \left(\frac{v}{P} \right) + \bar{s} \left(\frac{v}{P} \right)_\eta \right] \delta(x) \quad (19)$$

and substituting into equations (1) and (2), we obtain a simpler system, here expressed in terms of the more primitive functions

$$(\bar{J}')_\eta = u_\delta \frac{[\delta(x)]^2}{x} \frac{f(\eta)}{P(\eta)} \bar{s}_\eta - \frac{[\delta(x)]^2}{\rho_e c_e} [KFNO(\eta) - B(\eta) \bar{s} \bar{s}] + u_\delta \frac{[\delta(x)]^2}{P(\eta)} \eta^{1/2} \bar{s}_x \quad (20)$$

$$\bar{s}_\eta = \frac{\mp 11,600 \frac{\bar{D}(T)}{T(\eta)} \bar{s} \phi_\eta + P(\eta) \bar{J}'}{\bar{D}(T) + D_T(x, \eta)} \quad (21)$$

$$\phi_{\eta\eta} = - \frac{10^{14}}{8.85} en_e \frac{[\delta(x)]^2}{P(\eta)} (\bar{s}^+ - \bar{s}^-) \quad (22)$$

This transformation has two purposes: (1) to eliminate the need for derivatives of $f(\eta)/P(\eta)$ in the solution, and (2) to eliminate the singularity $\delta(x)/x$ at $x = 0$. This term now appears as $\delta^2/x = b^2 x^{0.6}$.

3. SMALL-VALUE, ASYMPTOTIC SOLUTIONS

Because of the fractional powers of x , a Taylor series solution does not exist at $x = 0$. In an attempt to find small-value (of x) solutions, we may eliminate the fractional powers in x by the transformation

$$t = x^{0.2} \text{ or } t^5 = x \quad (23)$$

with

$$\frac{dx}{dt} = 5t^4, \quad \frac{+}{s}_x = \frac{+}{s}_t \frac{dt}{dx} \quad (24)$$

and

$$\delta(x) = bt^4 \quad (25)$$

Equations (20) to (22) transform to

$$(\frac{+}{J'})_\eta = u_5 b^2 t^3 \frac{f(\eta)}{P(\eta)} \frac{+}{s}_\eta - \frac{b^2 t^8}{\rho_e c_e} [KFNO(\eta) - B(\eta) \frac{+}{s}s] + \frac{u_6 b^2 t^4 \eta^{1/8} \frac{+}{s}}{5P(\eta)} t \quad (26)$$

$$\frac{+}{s}_\eta = \frac{-11,600 \frac{\frac{+}{D}(T)}{T(\eta)} \frac{+}{s}\phi_\eta + P(\eta) \frac{+}{J'}}{\frac{+}{D}(T) + D_T(t^5, \eta)} \quad (27)$$

$$\phi_{\eta\eta} = -\frac{10^{14}}{8.85} en_e \frac{b^2 t^8}{P(\eta)} (\frac{+}{s} - \bar{s}) \quad (28)$$

A power series solution now takes the form

$$\frac{+}{J'} = \sum_{i=0}^{\infty} \frac{+}{J}_i(\eta) t^i \quad (29)$$

$$\frac{+}{s} = \sum_{i=0}^{\infty} \frac{+}{s}_i(\eta) t^i \quad (30)$$

$$\phi_\eta = \sum_{i=0}^{\infty} (\phi_\eta)_i(\eta) t^i \quad (31)$$

By substituting equations (29) to (31) into equations (26) to (28) and equating coefficients of powers of t , ordinary differential equations are found for the coefficients. [This procedure first requires a power series representation for $1/(\frac{+}{D} + D_T)$.] The smallest set of nonvanishing coefficients occurs for subscript 8 in equations (29) and (30) and subscript 16 in equation (31). We have

$$(\frac{+}{J}_8)_\eta = -\frac{b^2}{\rho_e c_e} KFNO(\eta) \quad (32)$$

$$(\frac{+}{s}_8)_\eta = \frac{P(\eta)}{\frac{+}{D}(T)} \frac{+}{J}_8 \quad (33)$$

$$[(\phi_\eta)_{16}]_\eta = -\frac{10^{14}}{8.85} en_e \frac{b^2}{P(\eta)} (\frac{+}{s}_8 - \bar{s}_8) \quad (34)$$

subject to the boundary conditions of equations (16) and (17); that is,
 $\bar{s}_g(0) = \bar{s}_g(0) = \bar{s}_g(1) = \bar{s}_g(1) = (\phi_\eta)_{16}(1) = 0$. Thus, we observe that for small t corresponding to small x ,

$$\bar{s}'(x, \eta) \approx \bar{s}_g(\eta)x^{1.6} \quad (35)$$

$$\bar{s}(x, \eta) \approx \bar{s}_g(\eta)x^{1.6} \quad (36)$$

$$\phi_\eta(x, \eta) \approx (\phi_\eta)_{16}(\eta)x^{3.2} \quad (37)$$

This analysis also suggests that ϕ_η is essentially decoupled from the equations for \bar{s} and \bar{s} for small x . The nonlinear term $\phi_\eta \bar{s}$ is negligible. In addition, the "+" and "-" equations are decoupled, since the nonlinear term $\bar{s}\bar{s}$ is negligible. These results are almost independent of the boundary conditions and must be considered when sets of boundary conditions are desired other than those given.

4. THE z, q TRANSFORMATION

The independent variables η and x are inconvenient variables to compute with. At $x = 0$, we have from equation (36) that $\bar{s}_x = 0$, but that \bar{s}_{xx} and higher derivatives are infinite. The finite difference scheme used to approximate \bar{s}_x from a sequence of values of \bar{s} is subject to large error when \bar{s}_{xxx} is large. Therefore, it is advantageous to use smaller intervals near $x = 0$ than are otherwise used. This situation is reinforced by the expected behavior of $\bar{s}_x \rightarrow 0$ as $x \rightarrow \infty$; the intervals in x can then be taken further apart. To accommodate both situations, we compute in a new variable z defined by

$$z = x^{0.8} \text{ or } x = z^{1.25} \quad (38)$$

mostly to simplify checking small-value results ($\bar{s} \sim z^2$) and provide for \bar{s}_{zz} to be finite. The equations are changed by replacing x by $z^{1.25}$ and

$$\frac{\bar{s}}{x} = \frac{\bar{s}}{z} \frac{dz}{dx} = \frac{0.8 \bar{s}_z}{z^{0.25}} \quad (39)$$

A similar, but more severe situation exists for the η independent variable. The driving function $KFNO(\eta)$ is monotonically decreasing and is almost an impulse function. For the Mach 8 data, $KFNO$ diminishes more than three orders of magnitude in the range $0 \leq \eta \leq 0.01$. It is essential in any finite difference scheme approximating derivatives with respect to η to have many intervals for small η . A transformation that automatically increases the number of η intervals for small η is given by

$$q = \ln(\eta + a) \quad (40)$$

where $a > 0$ is chosen to satisfy any particular requirement. In this case, a was chosen so that $\ln(a + 0.0001) - \ln(a)$ was equal to $1/400$ th of the total range of q . Equivalently, this assured that when 400 equal intervals were taken in the q direction, the first value of q corresponded to $\eta = 0$, and the second to $\eta = 0.0001$. The procedure was motivated by the fact that many of the input functions, including $KFNO(\eta)$, were constant for $0 \leq \eta \leq 0.0001$ and dropped off steeply thereafter. A special computer program computed $\ln(a) = -4.7939598$.

From equation (40), we have

$$\eta = e^q - a \quad (41)$$

$$\frac{d\eta}{dq} = e^q \quad (42)$$

This transformation is made by replacing η by $e^q - a$ [eq (41)] and replacing any variable r_η by

$$r_\eta = r_q \frac{dq}{d\eta} = \frac{r_q}{e^q} \quad (43)$$

In practice, the η notation was retained, except for derivatives with respect to η . All functions were computed as functions of η as found from equation (41) for any q . The transformed equations [from (20) to (22)] now appear as

$$\begin{aligned} \frac{(\dot{J}')}{e^q} = u_\delta \frac{\delta^2(z^{1.25}) f(\eta)}{e^q z^{1.25} P(\eta)} \frac{\dot{s}}{s} - \frac{\delta^2(z^{1.25})}{\rho e^c e} [KFNO(\eta) - B(\eta) \frac{\dot{s}}{s}] \\ + 0.8u_\delta \frac{\delta^2(z^{1.25}) \eta^{1/8}}{z^{0.25} P(\eta)} \frac{\dot{s}}{s} z \end{aligned} \quad (44)$$

$$\frac{\dot{s}_q}{e^q} = \frac{+11,600 \frac{\dot{D}(T)}{\dot{T}(\eta)} \frac{\dot{s}}{s} \phi_\eta + P(\eta) \dot{J}'}{\dot{D}(T) + D_T(z^{1.25}, \eta)} \quad (45)$$

$$\frac{(\phi_\eta)_q}{e^q} = - \frac{10^{14}}{8.85} e n_e \frac{\delta^2(z^{1.25})}{P(\eta)} (\dot{s} - \bar{s}) \quad (46)$$

with $\delta(z^{1.25}) = bz$.

5. NUMERICAL SOLUTION METHOD--LINEARIZATION

A "marching" technique is used to solve system (44) to (46) numerically. Given solutions at $z = z_{j-1}$, i.e., $\bar{s}(z_{j-1}, q)$, $\bar{J}'(z_{j-1}, q)$, and $\phi_\eta(z_{j-1}, q)$, ordinary differential equations in q are found at $z = z_j = z_{j-1} + \Delta z$ by an appropriate finite difference approximation for \bar{s}_z in terms of $\bar{s}(z_j, q)$, $\bar{s}(z_{j-1}, q)$, etc. To simplify notation hereafter, we refer to a function at fixed z_j with subscript j ; i.e., $\bar{s}(z_j, q) \equiv \bar{s}_j$, understanding that it is also a function of η .

The marching technique requires the solution of a two-point boundary-value problem with nonlinear differential equations. Although these can be solved directly by iterative processes, faster matrix algorithms can be used for linearized equations, which, at the same time, do not materially affect convergence characteristics. Accordingly, system (44) to (46) is linearized by deriving differential equations for changes in \bar{s}_{j-1} , \bar{J}'_{j-1} , and $(\phi_\eta)_{j-1}$. Defining

$$\bar{s}_j = \bar{s}_{j-1} + \Delta \bar{s}_j \quad (47)$$

$$\bar{J}'_j = \bar{J}'_{j-1} + \Delta \bar{J}'_j \quad (48)$$

$$(\phi_\eta)_j = (\phi_\eta)_{j-1} + (\Delta \phi_\eta)_j \quad (49)$$

we note that system (44) to (46) holds at both values of z_{j-1} and z_j . We substitute equations (47) to (49) into equations (44) to (46) and subtract from the resulting equations a similar set of equations obtained when \bar{s}_{j-1} , \bar{J}'_{j-1} , and $(\phi_\eta)_{j-1}$ are substituted into equations (44) to (46). This yields differential equations for $\Delta \bar{s}_j$, $\Delta \bar{J}'_j$, and $(\Delta \phi_\eta)_j$ with \bar{s}_{j-1} , \bar{J}'_{j-1} , and $(\phi_\eta)_{j-1}$ as additional input functions. The final equations, however, depend upon how the derivative \bar{s}_z is treated, as well as the nonlinear terms $\Delta \bar{s}_j (\Delta \phi_\eta)_j$ and $\Delta \bar{s}_j \Delta \bar{s}_j$.

A backward difference approximation² is used for \bar{s}_z when substituting at $z = z_j$:

$$\bar{s}_z = \frac{3\bar{s}_j - 4\bar{s}_{j-1} + \bar{s}_{j-2}}{2\Delta z} + O(\Delta z^2)$$

²Kcpal, Z., "Numerical Analysis," John Wiley & Sons, New York, 1955, pp. 515-516.

$$\bar{s}_z^+ = \frac{3\Delta\bar{s}_j^+ - \Delta\bar{s}_{j-1}^+}{2\Delta z} + O(\Delta z^2) \quad (50)$$

where $\bar{s}_{j-1}^+ = \bar{s}_{j-1}^+ - \bar{s}_{j-2}^+$, a quantity that must be stored during the computation. The appendage $O(\Delta z^2)$ indicates the approximation is of second order in Δz .

Equation (50) is not valid when $z = \Delta z$, i.e., for the first value of z , because $\Delta\bar{s}_0$ is nonexistent. Here, we use the condition that $\bar{s}_z = 0$ at $z = 0$. We may then show that the approximation becomes

$$\bar{s}_z^+ = \frac{2\Delta\bar{s}_1^+}{\Delta z} + O(\Delta z^2) \quad (51)$$

A central difference approximation is used for \bar{s}_z^+ when substituting at $z = z_{j-1}$

$$\begin{aligned} \bar{s}_z^+ &= \frac{\bar{s}_j^+ - \bar{s}_{j-2}^+}{2\Delta z} + O(\Delta z^2) \\ &= \frac{\Delta\bar{s}_j^+ + \Delta\bar{s}_{j-1}^+}{2\Delta z} + O(\Delta z^2) \end{aligned} \quad (52)$$

When $z = \Delta z$, we take $\bar{s}_z^+ = 0$ at $z = 0$, since it is a boundary condition.

Similarly, it is shown in appendix A that

$$\Delta\bar{s}_j^+(\Delta\phi_n)_j = 0 + O(\Delta z^2) \quad (53)$$

$$\Delta\bar{s}_j^+\Delta\bar{s}_j^- = 0 + O(\Delta z^2) \quad (54)$$

The substitution of equations (50) to (54) yields second-order computations of $\Delta\bar{s}_j^+$, ΔJ_j , and $(\Delta\phi_n)_j$ which, in turn, produce linear convergence in z for \bar{s} , J , and ϕ_n . (If Δz is halved, each $\Delta\bar{s}_j^+$, ΔJ_j , and $\Delta\phi_n$ is produced with one fourth the error, but there are then twice as many intervals to sum to reach a given z . Hence, if z is halved, the final error is only halved.) However, it was found that the error introduced by equations (53) and (54) was greater than that of equations (50) to (52). Accordingly, equations (53) and (54) were changed to (see appendix A)

$$\Delta\bar{s}_j^+(\Delta\phi_n)_j = \Delta\bar{s}_{j-1}^+(\Delta\phi_n)_j + O(\Delta z^3) \quad (55)$$

$$\Delta\bar{s}_j^+\Delta\bar{s}_j^- = \Delta\bar{s}_{j-1}^+(\Delta\bar{s})_j + O(\Delta z^3) \quad (56)$$

$$\text{or} \quad = \Delta\bar{s}_{j-1}^+(\Delta\bar{s})_j + O(\Delta z^3)$$

which still are linear terms in subscript j variables.

The final system of linear equations that must be solved for each j is given by (the subscript j is hereafter omitted to emphasize the dependent variables; $\Delta s \equiv \Delta s_j$, etc.):

$$e^{-q} \frac{d(\Delta \bar{s})}{dq} = \frac{1}{\bar{D}(\eta) + D_T(z_j^{1.25}, \eta)} \left\{ \bar{K}(\eta) \left[(\bar{s}_{j-1}^+ + \Delta \bar{s}_{j-1}^+) \Delta \phi_\eta + (\phi_\eta)_{j-1} \Delta \bar{s}^+ - \frac{\Delta D_T \bar{s}_{j-1}^+ (\phi_\eta)_{j-1}}{\bar{D}(\eta) + D_T(z_{j-1}^{1.25}, \eta)} \right] + P(\eta) \left[\Delta \bar{J} - (\bar{J}')_{j-1} \frac{\Delta D_T}{\bar{D}(\eta) + D_T(z_{j-1}^{1.25}, \eta)} \right] \right\} \quad (57)$$

$$e^{-q} \frac{d(\Delta \bar{J})}{dq} = u_\delta \frac{f(\eta)}{P(\eta)} \left[\frac{\delta_j^2}{z_j^{1.25}} \frac{\Delta \bar{s}_q^+}{e^q} + \Delta \left(\frac{\delta^2}{z^{1.25}} \right) \frac{(\bar{s}_q^+)_{j-1}}{e^q} \right] - \frac{KFNO(\eta) \Delta \delta^2}{\rho_e c_e} + \frac{B(\eta)}{\rho_e c_e} \left\{ \delta_j^2 \left[(\bar{s}_{j-1}^+ + \Delta \bar{s}_{j-1}^+) \Delta \bar{s} + \bar{s}_{j-1} \Delta \bar{s}^+ \right] + \Delta \delta^2 \bar{s}_{j-1}^+ \bar{s}_{j-1} \right\} + \frac{0.4u_\delta}{\Delta z} \frac{\eta^{1/8}}{P(\eta)} \left[\left(\frac{3\delta_j^2}{z_j^{0.25}} - \frac{\delta_{j-1}^2}{z_{j-1}^{0.25}} \right) \Delta \bar{s}^+ - \left(\frac{\delta_j^2}{z_j^{0.25}} + \frac{\delta_{j-1}^2}{z_{j-1}^{0.25}} \right) \Delta \bar{s}_{j-1}^+ \right] \quad (58)$$

$$e^{-q} \frac{d(\Delta \phi_\eta)}{dq} = - \frac{10^{14}}{8.85} \frac{en_e}{P(\eta)} \left[\delta_j^2 (\Delta \bar{s}^+ - \Delta \bar{s}) + \Delta \delta^2 (\bar{s}_{j-1}^+ - \bar{s}_{j-1}) \right] \quad (59)$$

where

$$\Delta D_T = 0.02 u_\delta \Delta z \eta^{1/8} \quad (60)$$

$$\Delta \left(\frac{\delta^2}{z^{1.25}} \right) = \frac{\delta_j^2}{z_j^{1.25}} - \frac{\delta_{j-1}^2}{z_{j-1}^{1.25}} \quad (61)$$

$$\Delta \delta^2 = \delta_j^2 - \delta_{j-1}^2 \quad (62)$$

If $\Delta \bar{s}_0^+$ is initially set equal to 0, the correct formulas are obtained when $j = 1$ if the term $3\delta_j^2/z_j^{0.25}$ is changed to $4\delta_j^2/z_j^{0.25}$ in equation (58).

It should be emphasized that quadratic convergence in Δz can be obtained if all approximations are such that the $\Delta \bar{s}_i^{\pm}$, ΔJ_i^{\pm} , and $\Delta \phi_{\eta i}$ are computed with order Δz^3 . Although this was not done, appendix B indicates the changes required.

5.1 Matrix Formulation

If a grid of $N + 1$ equally-spaced points is placed along q , starting at q_1 corresponding to $\eta = 0$ and ending at q_{N+1} corresponding to $\eta = 1$, we may correspond to these points $5(N + 1)$ functional values we seek. Thus, for every j , we seek for all i , $1 \leq i \leq N + 1$ the values $\Delta \bar{s}_i^{\pm}$, ΔJ_i^{\pm} , and $(\Delta \phi_{\eta})_i$. Approximate values may be found with second-order error in Δq by satisfying equations (57) to (62) at the half-interval stations by using the approximations

$$(r_q)_{i+1/2} = \frac{r_{i+1} - r_i}{\Delta q} + O(\Delta q^2) \quad 1 \leq i \leq N \quad (63)$$

$$r_{i+1/2} = \frac{r_{i+1} + r_i}{2} + O(\Delta q^2) \quad 1 \leq i \leq N \quad (64)$$

where r is any required variable or stored variable at $j - 1$. This results in $5N$ linear algebraic equations, which, coupled with the five boundary conditions of equations (16) and (17), may be solved for the $5N + 5$ functional values. By incrementing z_j , storing the required $\Delta \bar{s}$ at each i (to be the new set of Δs_{j-1}), and mechanizing equations (47) to (49), the procedure may be used to reach any desired value of z .

5.2 Computer Solution

The computer program is written to accommodate any set of feasible boundary conditions, since this was one uncertain aspect at the time of development. It is important to prearrange the equations so that their final matrix form has a matrix coefficient that is block-tridiagonal (each block a 5×5 square matrix), in order to use an efficient algorithm³ for their solution. A difficulty in doing this is the uncertainty of where the boundary conditions will be imposed. There must be five conditions, but m of these will be at $\eta = 0$ and $5 - m$ at $\eta = 1$.

³Isaacson, E. and Keller, H.B., "Analysis of Numerical Methods," John Wiley & Sons, New York, 1966, pp. 58-61.

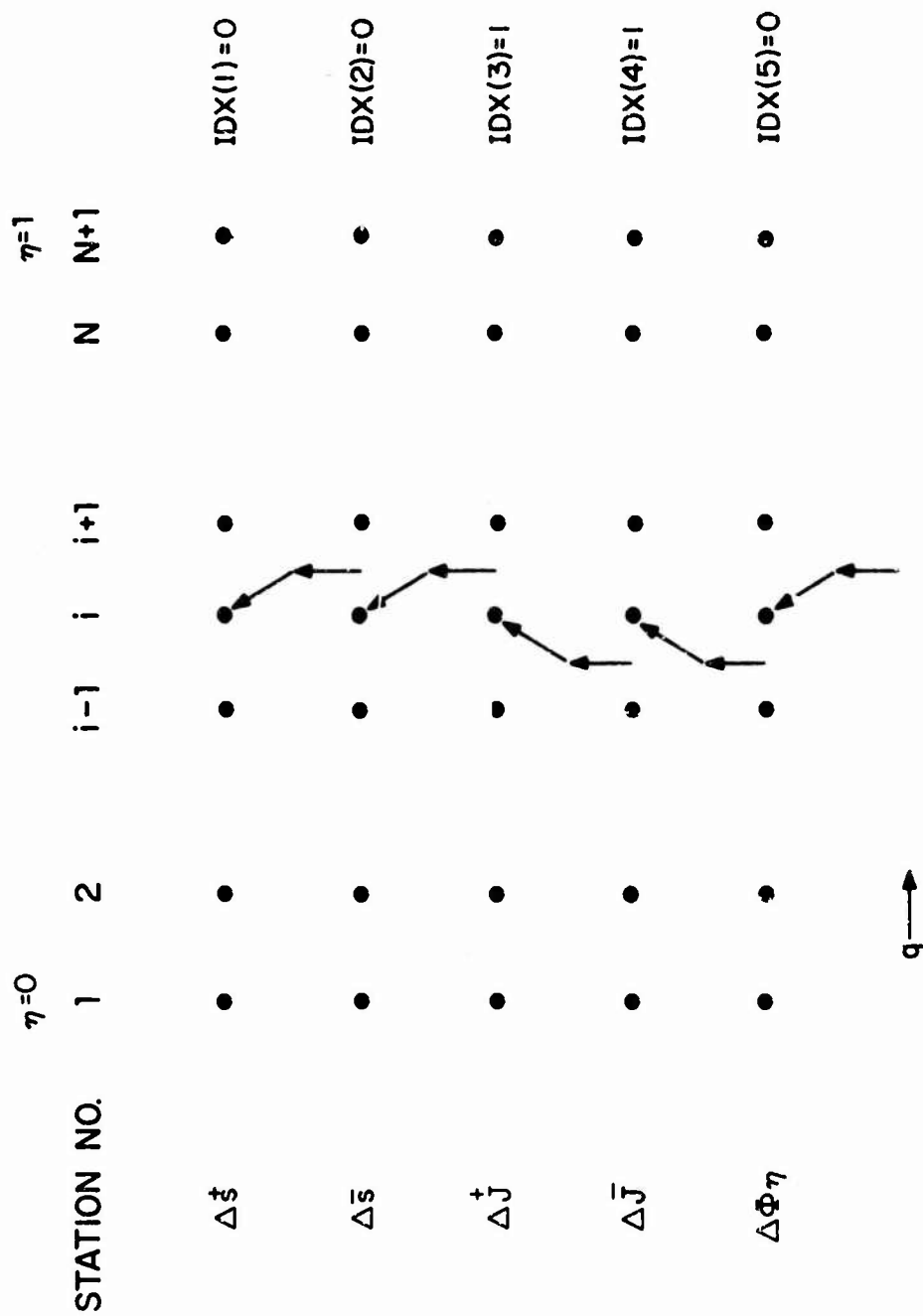


Figure 1. Scheme for matrix generation.

5.3 Solution Checks

A separate program, COMPF (not included here), computed $f(\eta)$ using equation (14) from the $P(\eta)$ data fed in, and punched the data out in the proper format. It utilized a standard integration routine; the final results were checked approximately by Simpson's rule for the Mach 8 data. Thereafter, the program was assumed correct for other data.

Another separate program, FTEST (also not listed here), checked out the FUNCT subroutine listed in appendix C. This was important to insure that all functions of η were properly generated and stored for use in the main body of the program. Included was a printout utilizing the stored functions. Points were spot checked in each column to insure reasonableness. The printout for the Mach 10 data is shown in table I.

In addition to the printout of all functions, graphs of the functions were plotted against η using HDL's CalComp plotting equipment by another specially written subprogram GRAPHS. In this way, gross errors or any disturbance from the quadratic interpolation of the input data could be easily detected. Examples of the graphs are shown in figure 2.

The major check on the validity of the results was a separate independent program, POLCHK, which solved system (57) to (59) directly with the aid of a differential-equation-solving subroutine FNOL2. Solutions of two-point boundary-value problems require no iteration with linear differential equations. Let the vector-matrix differential equation be

$$A(\eta) \frac{dx}{d\eta} = g(\eta) \quad (66)$$

with $x_1 = \Delta s^+$, $x_2 = \Delta s^-$, $x_3 = \Delta J^+$, $x_4 = \Delta J^-$, and $x_5 = \Delta \delta_\eta$. We start at $\eta = 1$ and run solutions with decreasing η , using the known initial (at $\eta = 1$) conditions $x_1(1) = 0$, $x_2(1) = 0$, and $x_5(1) = 0$. The other conditions vary in each of the three separate solutions:

$$A(\eta) \frac{dp}{d\eta} = g(\eta), \quad p_3 = d_1, \quad p_4 = 0 \quad (67)$$

$$A(\eta) \frac{dq}{d\eta} = g(\eta), \quad q_3 = 0, \quad q_4 = d_2 \quad (68)$$

$$A(\eta) \frac{dr}{d\eta} = g(\eta), \quad r_3 = d_1, \quad r_4 = d_2 \quad (69)$$

where $p_k(1) = q_k(1) = r_k(1) = x_k(1) = 0$ when $k = 1, 2$, or 5 .

Because of the superposition theorem, it is easily shown that

$$x = ap + bq + cr, \quad (70)$$

if and only if

Table I. FREST output for Mach 10 data.

V = 3.35249E 05 C = 0.0200 RHOICE = 5.5300E 12 NE = 5.6300E 12 DT FACTOR = 5710.

ETA	P	T	F	KFO	N	CLPLUS	KPLUS	BLMINUS	RMINUS	ETAP.125	ETAP.125
4.935E-05	1.000E-00	3.672E-00	03-1.156E-05	2.894E-17	4.273E-17	2.359E-00	7.453E-00	5.521E-00	1.744E-03	2.897E-01	1.440E-05
2.395E-04	9.503E-01	3.540E-00	03-2.838E-04	1.003E-16	4.994E-17	2.224E-00	7.281E-00	5.201E-00	1.703E-03	4.155E-01	3.096E-04
1.814E-03	9.330E-01	3.444E-00	03-5.325E-03	5.281E-16	5.310E-17	2.155E-00	7.209E-00	5.067E-00	1.637E-03	4.542E-01	8.239E-04
2.431E-03	9.153E-01	3.342E-00	03-1.027E-02	3.249E-16	5.593E-17	2.115E-00	7.171E-00	4.949E-00	1.672E-03	4.809E-01	1.258E-03
3.751E-03	8.902E-01	3.244E-00	03-1.478E-02	2.131E-16	5.953E-17	2.059E-00	7.027E-00	4.839E-00	1.658E-03	5.101E-01	1.978E-03
2.164E-03	8.473E-01	3.047E-00	03-1.923E-02	1.608E-16	6.527E-17	2.039E-00	7.027E-00	4.752E-00	1.646E-03	5.101E-01	2.665E-03
2.542E-03	8.730E-01	3.211E-00	03-2.560E-02	1.176E-16	6.507E-17	1.994E-00	6.987E-00	4.657E-00	1.635E-03	5.332E-01	3.494E-03
4.039E-03	8.683E-01	3.278E-00	03-3.223E-02	5.629E-16	6.789E-17	1.964E-00	6.943E-00	4.589E-00	1.624E-03	5.471E-01	3.370E-03
4.513E-03	8.683E-01	3.278E-00	03-3.223E-02	5.629E-16	6.789E-17	1.964E-00	6.943E-00	4.589E-00	1.624E-03	5.471E-01	3.370E-03
1.491E-02	8.457E-01	3.215E-00	03-4.777E-02	4.517E-16	7.272E-17	1.894E-00	6.844E-00	4.459E-00	1.602E-03	5.729E-01	4.571E-03
1.398E-02	8.364E-01	3.184E-00	03-5.683E-02	3.210E-16	7.584E-17	1.864E-00	6.804E-00	4.359E-00	1.592E-03	5.835E-01	7.871E-03
1.588E-02	8.265E-01	3.151E-00	03-6.697E-02	2.242E-16	7.866E-17	1.834E-00	6.764E-00	4.259E-00	1.580E-03	5.946E-01	9.321E-03
1.831E-02	8.163E-01	3.117E-00	03-7.815E-02	1.565E-16	8.148E-17	1.804E-00	6.724E-00	4.159E-00	1.568E-03	6.050E-01	1.095E-02
2.071E-02	8.061E-01	3.083E-00	03-9.064E-02	1.036E-16	8.430E-17	1.774E-00	6.684E-00	4.059E-00	1.556E-03	6.150E-01	1.274E-02
2.306E-02	7.959E-01	3.049E-00	03-1.047E-01	7.134E-16	8.713E-17	1.744E-00	6.644E-00	3.959E-00	1.544E-03	6.250E-01	1.461E-02
2.542E-02	7.857E-01	3.015E-00	03-1.201E-01	4.738E-16	9.025E-17	1.714E-00	6.604E-00	3.859E-00	1.532E-03	6.350E-01	1.658E-02
2.777E-02	7.755E-01	2.981E-00	03-1.375E-01	3.030E-16	9.337E-17	1.684E-00	6.564E-00	3.759E-00	1.520E-03	6.450E-01	1.865E-02
3.012E-02	7.653E-01	2.947E-00	03-1.557E-01	1.872E-16	9.650E-17	1.654E-00	6.524E-00	3.659E-00	1.508E-03	6.550E-01	2.072E-02
3.247E-02	7.551E-01	2.913E-00	03-1.752E-01	1.117E-16	9.963E-17	1.624E-00	6.484E-00	3.559E-00	1.496E-03	6.650E-01	2.279E-02
3.482E-02	7.449E-01	2.879E-00	03-1.960E-01	6.731E-16	1.030E-16	1.594E-00	6.444E-00	3.459E-00	1.484E-03	6.750E-01	2.486E-02
3.717E-02	7.347E-01	2.845E-00	03-2.241E-01	3.915E-16	1.117E-16	1.564E-00	6.404E-00	3.359E-00	1.472E-03	6.850E-01	2.693E-02
3.952E-02	7.245E-01	2.811E-00	03-2.512E-01	2.147E-16	1.204E-16	1.534E-00	6.364E-00	3.259E-00	1.460E-03	6.950E-01	2.900E-02
4.187E-02	7.143E-01	2.777E-00	03-2.811E-01	1.162E-16	1.291E-16	1.504E-00	6.324E-00	3.159E-00	1.448E-03	7.050E-01	3.107E-02
4.422E-02	7.041E-01	2.743E-00	03-3.139E-01	5.652E-16	1.378E-16	1.474E-00	6.284E-00	3.059E-00	1.436E-03	7.150E-01	3.314E-02
4.657E-02	6.939E-01	2.709E-00	03-3.487E-01	2.561E-16	1.465E-16	1.444E-00	6.244E-00	2.959E-00	1.424E-03	7.250E-01	3.521E-02
4.892E-02	6.837E-01	2.675E-00	03-3.879E-01	1.534E-16	1.552E-16	1.414E-00	6.204E-00	2.859E-00	1.412E-03	7.350E-01	3.728E-02
5.127E-02	6.735E-01	2.641E-00	03-4.296E-01	4.784E-16	1.640E-16	1.384E-00	6.164E-00	2.759E-00	1.400E-03	7.450E-01	3.935E-02
5.362E-02	6.633E-01	2.607E-00	03-4.746E-01	1.741E-16	1.728E-16	1.354E-00	6.124E-00	2.659E-00	1.388E-03	7.550E-01	4.142E-02
5.597E-02	6.531E-01	2.573E-00	03-5.237E-01	6.016E-16	1.816E-16	1.324E-00	6.084E-00	2.559E-00	1.376E-03	7.650E-01	4.349E-02
5.832E-02	6.429E-01	2.539E-00	03-5.769E-01	3.329E-16	1.904E-16	1.294E-00	6.044E-00	2.459E-00	1.364E-03	7.750E-01	4.556E-02
6.067E-02	6.327E-01	2.505E-00	03-6.349E-01	1.868E-16	1.992E-16	1.264E-00	6.004E-00	2.359E-00	1.352E-03	7.850E-01	4.763E-02
6.302E-02	6.225E-01	2.471E-00	03-6.979E-01	8.672E-16	2.080E-16	1.234E-00	5.964E-00	2.259E-00	1.340E-03	7.950E-01	4.970E-02
6.537E-02	6.123E-01	2.437E-00	03-7.669E-01	3.039E-16	2.168E-16	1.204E-00	5.924E-00	2.159E-00	1.328E-03	8.050E-01	5.177E-02
6.772E-02	6.021E-01	2.403E-00	03-8.419E-01	1.541E-16	2.256E-16	1.174E-00	5.884E-00	2.059E-00	1.316E-03	8.150E-01	5.384E-02
7.007E-02	5.919E-01	2.369E-00	03-9.239E-01	6.075E-16	2.344E-16	1.144E-00	5.844E-00	1.959E-00	1.304E-03	8.250E-01	5.591E-02
7.242E-02	5.817E-01	2.335E-00	03-1.013E-01	2.472E-16	2.432E-16	1.114E-00	5.804E-00	1.859E-00	1.292E-03	8.350E-01	5.798E-02
7.477E-02	5.715E-01	2.301E-00	03-1.101E-01	1.541E-16	2.520E-16	1.084E-00	5.764E-00	1.759E-00	1.280E-03	8.450E-01	6.005E-02
7.712E-02	5.613E-01	2.267E-00	03-1.199E-01	7.511E-16	2.608E-16	1.054E-00	5.724E-00	1.659E-00	1.268E-03	8.550E-01	6.212E-02
7.947E-02	5.511E-01	2.233E-00	03-1.307E-01	3.298E-16	2.696E-16	1.024E-00	5.684E-00	1.559E-00	1.256E-03	8.650E-01	6.419E-02
8.182E-02	5.409E-01	2.200E-00	03-1.425E-01	1.945E-16	2.784E-16	9.94E-01	5.644E-00	1.459E-00	1.244E-03	8.750E-01	6.626E-02
8.417E-02	5.307E-01	2.166E-00	03-1.553E-01	7.511E-16	2.872E-16	9.64E-01	5.604E-00	1.359E-00	1.232E-03	8.850E-01	6.833E-02
8.652E-02	5.205E-01	2.132E-00	03-1.691E-01	3.607E-16	2.960E-16	9.34E-01	5.564E-00	1.259E-00	1.220E-03	8.950E-01	7.040E-02
8.887E-02	5.103E-01	2.098E-00	03-1.839E-01	1.608E-16	3.048E-16	9.04E-01	5.524E-00	1.159E-00	1.208E-03	9.050E-01	7.247E-02
9.122E-02	5.001E-01	2.064E-00	03-1.997E-01	7.511E-16	3.136E-16	8.74E-01	5.484E-00	1.059E-00	1.196E-03	9.150E-01	7.454E-02
9.357E-02	4.899E-01	2.030E-00	03-2.165E-01	3.607E-16	3.224E-16	8.44E-01	5.444E-00	959E-00	1.184E-03	9.250E-01	7.661E-02
9.592E-02	4.797E-01	1.996E-00	03-2.343E-01	1.608E-16	3.312E-16	8.14E-01	5.404E-00	859E-00	1.172E-03	9.350E-01	7.868E-02
9.827E-02	4.695E-01	1.962E-00	03-2.531E-01	7.511E-16	3.400E-16	7.84E-01	5.364E-00	759E-00	1.160E-03	9.450E-01	8.075E-02
1.0062E-01	4.593E-01	1.928E-00	03-2.729E-01	3.607E-16	3.488E-16	7.54E-01	5.324E-00	659E-00	1.148E-03	9.550E-01	8.282E-02
1.0297E-01	4.491E-01	1.894E-00	03-2.937E-01	1.608E-16	3.576E-16	7.24E-01	5.284E-00	559E-00	1.136E-03	9.650E-01	8.489E-02
1.0532E-01	4.389E-01	1.860E-00	03-3.155E-01	7.511E-16	3.664E-16	6.94E-01	5.244E-00	459E-00	1.124E-03	9.750E-01	8.696E-02
1.0767E-01	4.287E-01	1.826E-00	03-3.383E-01	3.607E-16	3.752E-16	6.64E-01	5.204E-00	359E-00	1.112E-03	9.850E-01	8.903E-02
1.1002E-01	4.185E-01	1.792E-00	03-3.621E-01	1.608E-16	3.840E-16	6.34E-01	5.164E-00	259E-00	1.100E-03	9.950E-01	9.110E-02
1.1237E-01	4.083E-01	1.758E-00	03-3.869E-01	7.511E-16	3.928E-16	6.04E-01	5.124E-00	159E-00	1.088E-03	1.000E-01	9.317E-02
1.1472E-01	3.981E-01	1.724E-00	03-4.127E-01	3.607E-16	4.016E-16	5.74E-01	5.084E-00	59E-00	1.076E-03	1.100E-01	9.524E-02
1.1707E-01	3.879E-01	1.690E-00	03-4.395E-01	1.608E-16	4.104E-16	5.44E-01	5.044E-00	00	1.064E-03	1.200E-01	9.731E-02
1.1942E-01	3.777E-01	1.656E-00	03-4.673E-01	7.511E-16	4.192E-16	5.14E-01	5.004E-00	00	1.052E-03	1.300E-01	9.938E-02
1.2177E-01	3.675E-01	1.622E-00	03-4.961E-01	3.607E-16	4.280E-16	4.84E-01	4.964E-00	00	1.040E-03	1.400E-01	1.014E-01
1.2412E-01	3.573E-01	1.588E-00	03-5.259E-01	1.608E-16	4.368E-16	4.54E-01	4.924E-00	00	1.028E-03	1.500E-01	1.034E-01
1.2647E-01	3.471E-01	1.554E-00	03-5.567E-01	7.511E-16	4.456E-16	4.24E-01	4.884E-00	00	1.016E-03	1.600E-01	1.054E-01
1.2882E-01	3.369E-01	1.520E-00	03-5.885E-01	3.607E-16	4.544E-16	3.94E-01	4.844E-00	00	1.004E-03	1.700E-01	1.074E-01
1.3117E-01	3.267E-01	1.486E-00	03-6.213E-01	1.608E-16	4.632E-16	3.64E-01	4.804E-00	00	9.92E-04	1.800E-01	1.094E-01
1.3352E-01	3.165E-01	1.452E-00	03-6.551E-01	7.511E-16	4.720E-16	3.34E-01	4.764E-00	00	9.80E-04	1.900E-01	1.114E-01
1.3587E-01	3.063E-01	1.418E-00	03-6.899E-01	3.607E-16	4.808E-16	3.04E-01	4.724E-00	00	9.68E-04	2.000E-01	1.134E-01
1.3822E-01	2.961E-01	1.384E-00	03-7.257E-01	1.608E-16	4.896E-16	2.74E-01	4.684E-00	00	9.56E-04	2.100E-01	1.154E-01
1.4057E-01	2.859E-01	1.350E-00	03-7.625E-01	7.511E-16	4.984E-16	2.44E-01	4.644E-00	00	9.44E-04	2.200E-01	1.174E-01
1.4292E-01	2.757E-01	1.316E-00	03-8.003E-01	3.607E-16	5.072E-16	2.14E-01	4.604E-00	00	9.32E-04	2.300E-01	1.194E-01
1.4527E-01	2.655E-01	1.282E-00	03-8.391E-01	1.608E-16	5.160E-16	1.84E-01	4.564E-00	00	9.20E-04	2.400E-01	1.214E-01
1.4762E-01	2.553E-01	1.248E-00	03-8.789E-01	7.511E-16	5.248E-16	1.54E-01	4.524E-00	00	9.08E-04	2.500E-01	1.234E-01
1.4997E-01	2.451E-01	1.214E-00	03-9.197E-01	3.607E-16	5.336E-16	1.24E-01	4.484E-00	00	8.96E-04	2.600E-01	1.254E-01
1.5232E-01	2.349E-01	1.180E-00	03-9.615E-01	1.608E-16	5.424E-16	9.4E-02					

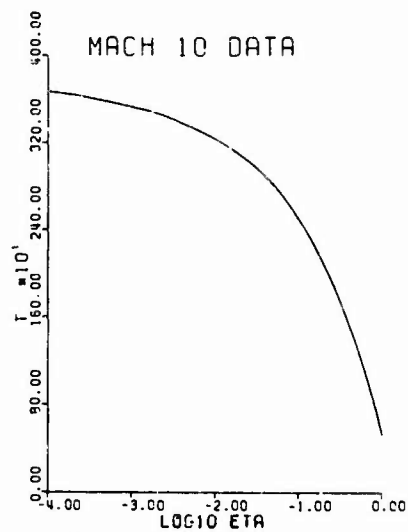
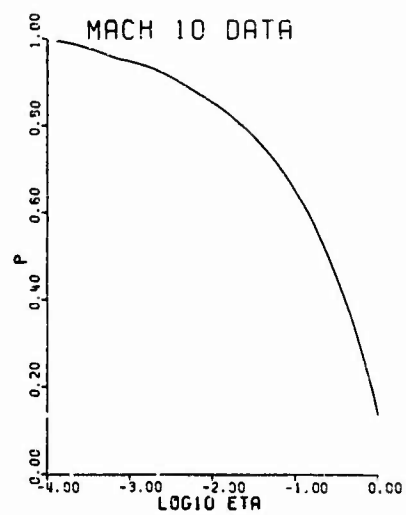
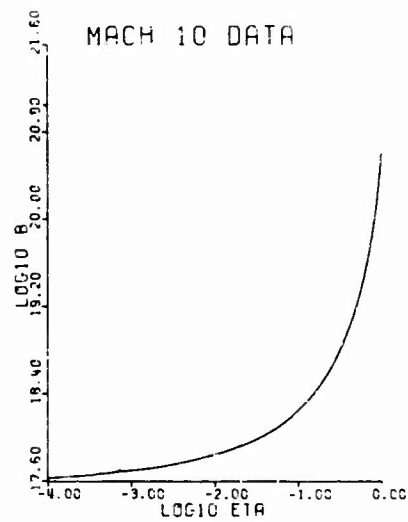
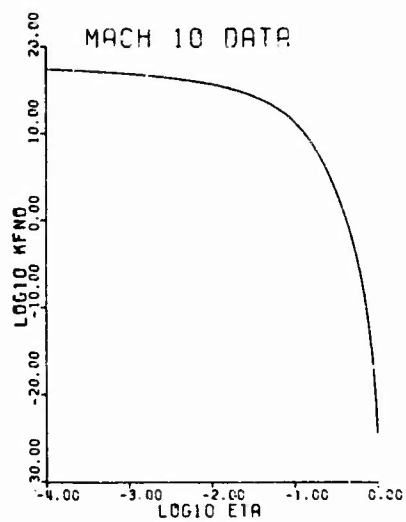
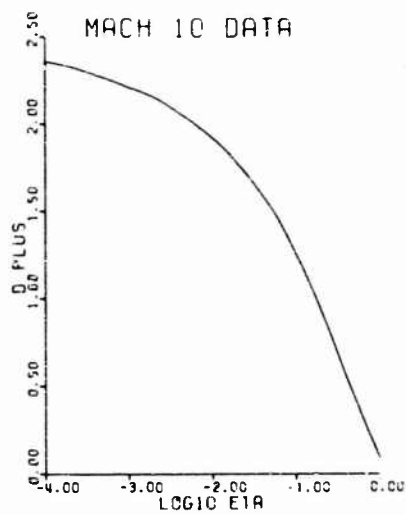
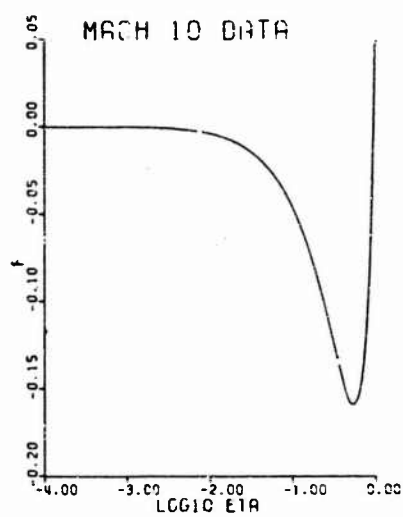


Figure 2. GRAPHS output.

$$a + b + c = 1, \quad (71)$$

and the boundary conditions are satisfied:

$$\Delta \bar{s}^+(0) = x_1(0) = ap_1(0) + bq_1(0) + cr_1(0) = 0 \quad (72)$$

$$\Delta \bar{s}^-(0) = x_2(0) = ap_2(0) + bq_2(0) + cr_2(0) = 0. \quad (73)$$

Equations (71) to (73) can be solved for a , b , and c . The initial conditions d_1 and d_2 can be arbitrarily nonzero, but in practice they are chosen so that $r(\eta)$ is close to $x(\eta)$; i.e., c will be very nearly equal to 1. This minimizes roundoff errors since the magnitudes of a , b , and c can otherwise be quite large but of opposite sign. The program was written so that d_1 and d_2 were iterated on successive runs h and $h + 1$ before z was stepped up:

$$(d_1)_{h+1} = (d_1)_h (a + c) \quad (74)$$

$$(d_2)_{h+1} = (d_2)_h (b + c) \quad (75)$$

The iteration was stopped when the magnitudes a and b were appropriately small enough. Theoretically, c at step 3 should equal c at step 2 exactly, but because of roundoff errors and the inability to exactly solve differential equations numerically, the iteration index occasionally went to 4.

A fourth-order Runge-Kutta integration scheme was used to compute the values of variables at fixed points. These points were sufficiently close, so that error in the η direction was essentially negligible. This check showed that the finite difference scheme of section 5.2 was working correctly, and that the error introduced in the η direction was less than 2 percent when using 400 intervals (for Mach 8 data).

By obtaining runs at a given Δz , $\Delta z/2$, and $\Delta z/4$, the linear nature of the convergence in the z direction was verified. In addition, the error using

$$\Delta z = \frac{100^{0.8}}{50} = \frac{z_{\max}}{50}$$

was less than 5 percent (for Mach 10 data). Such a run corresponded to about 8 minutes of IBM 7094 CPU time.

Appendix A. Order of Errors in Nonlinear Approximations

Since

$$\frac{\pm}{s} = \frac{\pm}{s}_{j-1} + \left(\frac{\partial \frac{\pm}{s}}{\partial z} \right)_{j-1} (z - z_{j-1}) + \frac{1}{2} \left(\frac{\partial^2 \frac{\pm}{s}}{\partial z^2} \right)_{j-1} (z - z_{j-1})^2 + \dots$$

we have

$$\frac{\pm}{s}_j - \frac{\pm}{s}_{j-1} = \Delta \frac{\pm}{s}_j = \left(\frac{\partial \frac{\pm}{s}}{\partial z} \right)_{j-1} \Delta z + \frac{1}{2} \left(\frac{\partial^2 \frac{\pm}{s}}{\partial z^2} \right)_{j-1} \Delta z^2 + \dots$$

Similarly,

$$(\Delta \phi_\eta)_j = \left(\frac{\partial \phi_\eta}{\partial z} \right)_{j-1} \Delta z + \frac{1}{2} \left(\frac{\partial^2 \phi_\eta}{\partial z^2} \right)_{j-1} \Delta z^2 + \dots$$

so that

$$\Delta \frac{\pm}{s}_j (\Delta \phi_\eta)_j = \left(\frac{\partial \frac{\pm}{s}}{\partial z} \right)_{j-1} \left(\frac{\partial \phi_\eta}{\partial z} \right)_{j-1} \Delta z^2 + \dots$$

$$= 0 + O(\Delta z^2)$$

$$\Delta \frac{\pm}{s}_j \Delta \bar{s}_j = \left(\frac{\partial \frac{\pm}{s}}{\partial z} \right)_{j-1} \left(\frac{\partial \bar{s}}{\partial z} \right)_{j-1} \Delta z^2 + \dots$$

$$= 0 + O(\Delta z^2)$$

This implies that ignoring the nonlinear terms simply introduces a second-order error. On the other hand, we also have

$$\Delta \frac{\pm}{s}_{j-1} = \left(\frac{\partial \frac{\pm}{s}}{\partial z} \right)_{j-2} \Delta z + \frac{1}{2} \left(\frac{\partial^2 \frac{\pm}{s}}{\partial z^2} \right)_{j-2} \Delta z^2 + \dots$$

so that by subtracting

$$\Delta \frac{\pm}{s}_j - \Delta \frac{\pm}{s}_{j-1} = \left[\left(\frac{\partial \frac{\pm}{s}}{\partial z} \right)_{j-1} - \left(\frac{\partial \frac{\pm}{s}}{\partial z} \right)_{j-2} \right] \Delta z + \frac{1}{2} \left[\left(\frac{\partial^2 \frac{\pm}{s}}{\partial z^2} \right)_{j-1} - \left(\frac{\partial^2 \frac{\pm}{s}}{\partial z^2} \right)_{j-2} \right] \Delta z^2 + \dots$$

But,

$$\frac{\partial \frac{\pm}{s}}{\partial z} = \left(\frac{\partial \frac{\pm}{s}}{\partial z} \right)_{j-1} + \left(\frac{\partial^2 \frac{\pm}{s}}{\partial z^2} \right)_{j-1} (z - z_{j-1}) + \dots$$

so that

$$\left(\frac{\partial \frac{\pm}{s}}{\partial z} \right)_{j-1} - \left(\frac{\partial \frac{\pm}{s}}{\partial z} \right)_{j-2} = \left(\frac{\partial^2 \frac{\pm}{s}}{\partial z^2} \right)_{j-1} \Delta z + \dots$$

This leads to

$$\Delta \bar{s}_j^+ = \Delta \bar{s}_{j-1}^+ + O(\Delta z^2)$$

and

$$\Delta \bar{s}_j^+ (\Delta \phi_n)_j = \Delta \bar{s}_{j-1}^+ (\Delta \phi_n)_j + O(\Delta z^3)$$

Equation (56) follows similarly. Since $\Delta \bar{s}_{j-1}^+$ must be stored for the derivative approximation equation (50) anyway, no additional storage is required.

Appendix B. Formulas for Quadratic Convergence in z

The first set of $\Delta \bar{s}_1$, ΔJ , and $\Delta \phi_\eta$ can be computed with a second-order error, but each set thereafter should be computed with third-order to obtain quadratic convergence. No change, therefore, occurs for $j = 1$; equation (51) applies for the \bar{s}_z approximation at $z = \Delta z$.

For $j = 2$, i.e., $z = 2\Delta z$, a special computation must be made, taking into account the stored $\Delta \bar{s}_1$ and the fact that $\bar{s}_z = 0$ at $z = 0$. Note that we need to estimate \bar{s}_z at $z = \Delta z$ as well as $z = 2\Delta z$. If $z = z_1 (= \Delta z)$, we set up a Taylor expansion of $s(z)$ about z_1 .

$$s = s_1 + s'_1(z - z_1) + \frac{1}{2} s''_1(z - z_1)^2 + \frac{1}{6} s'''_1(z - z_1)^3 + \frac{1}{24} s''''_1(z - z_1)^4 + \dots$$

$$s' = s'_1 + s''_1(z - z_1) + \frac{1}{2} s'''_1(z - z_1)^2 + \frac{1}{6} s''''_1(z - z_1)^3 + \dots$$

At $z = z_1 - \Delta z (= z_0 = 0)$, $s = 0$ and $s' = 0$. Also, at $z = z_1 + \Delta z = z_2$, $s = s_2$. Thus,

$$0 = s_0 = s_1 - s'_1 \Delta z + \frac{1}{2} s''_1 \Delta z^2 - \frac{1}{6} s'''_1 \Delta z^3 + \frac{1}{24} s''''_1 \Delta z^4 + \dots$$

$$0 = s'_1 - s''_1 \Delta z + \frac{1}{2} s'''_1 \Delta z^2 - \frac{1}{6} s''''_1 \Delta z^3 + \dots$$

$$s_2 = s_1 + s'_1 \Delta z + \frac{1}{2} s''_1 \Delta z^2 + \frac{1}{6} s'''_1 \Delta z^3 + \frac{1}{24} s''''_1 \Delta z^4 + \dots$$

Eliminating s''_1 and s'''_1 from the equations yields

$$s'_1 = \frac{4s_1 + s_2}{4\Delta z} - \frac{s''''_1}{24} \Delta z^3 + \dots$$

or, in terms of Δs_2 and Δs_1 ,

$$s'_1 = \frac{5\Delta s_1 + \Delta s_2}{4\Delta z} + O(\Delta z^3)$$

since $s_2 - s_1 = \Delta s_2$ and $s_1 = \Delta s_1$.

To find s'_2 in terms of Δs_1 and Δs_2 , a Taylor series about $z = z_2$ is constructed:

$$s = s_2 + s'_2(z - z_2) + \frac{1}{2} s''_2(z - z_2)^2 + \frac{1}{6} s'''_2(z - z_2)^3 + \frac{1}{24} s''''_2(z - z_2)^4 + \dots$$

with

$$s' = s_2' + s_2''(z - z_2) + \frac{1}{2} s_2'''(z - z_2)^2 + \frac{1}{6} s_2''''(z - z_2)^3 + \dots$$

At $z = 0$ ($z - z_2 = -2\Delta z$), $s = s' = 0$, and at $z = z_1$, $s = s_1$. Thus,

$$0 = s_2 - 2s_2'\Delta z + 2s_2''\Delta z^2 - \frac{8}{6} s_2'''\Delta z^3 + \frac{16}{24} s_2''''\Delta z^4 + \dots$$

$$0 = s_2' - 2s_2''\Delta z + 2s_2'''\Delta z^2 - \frac{8}{6} s_2''''\Delta z^3 + \dots$$

$$s_1 = s_2 - s_2'\Delta z + \frac{1}{2} s_2''\Delta z^2 - \frac{1}{6} s_2'''\Delta z^3 + \frac{1}{24} s_2''''\Delta z^4 + \dots$$

Eliminating s_2'' and s_2''' from the equations yields

$$s_2' = \frac{2s_2 - s_1}{\Delta z} + \frac{1}{6} s_2''''\Delta z^3 + \dots$$

In terms of Δs_2 and Δs_1 ,

$$s_2' = \frac{2\Delta s_2 - 2\Delta s_1}{\Delta z} + O(\Delta z^3)$$

A projected Δs_j for use in the nonlinear approximations (55) and (56) can also be found by eliminating s_2' and s_2'' from the above equations. We have

$$s_2 = 4s_1 + \frac{2}{3} s_2'''\Delta z^3 + \dots$$

or

$$\Delta s_2 = 3\Delta s_1 + O(\Delta z^3)$$

From appendix A,

$$\Delta \bar{s}_2^+(\Delta \phi_\eta)_2 = 3\Delta \bar{s}_1^+(\Delta \phi_\eta)_2 + O(\Delta z^4)$$

$$\Delta \bar{s}_2^+\Delta \bar{s}_2^- = 3\Delta \bar{s}_1^+\Delta \bar{s}_2^- + O(\Delta z^4)$$

$$\text{or} \quad = 3\Delta \bar{s}_2^+\Delta \bar{s}_1^- + O(\Delta z^4)$$

For $j \geq 3$, we may use standard formulas²

$$s_{j-1}' = \frac{s_{j-3} - 6s_{j-2} + 3s_{j-1} + 2s_j}{6\Delta z} + O(\Delta z^3)$$

²Kopal, Z., "Numerical Analysis," John Wiley & Sons, New York, 1955, pp. 515-516.

or

$$s'_{j-1} = \frac{2\Delta s_j + 5\Delta s_{j-1} - \Delta s_{j-2}}{6\Delta z} + O(\Delta z^3)$$

and

$$s'_j = \frac{-2s_{j-3} + 9s_{j-2} - 18s_{j-1} + 11s_j}{6\Delta z} + O(\Delta z^3)$$

or

$$s'_j = \frac{11\Delta s_j - 7\Delta s_{j-1} + 2\Delta s_{j-2}}{6\Delta z} + O(\Delta z^3)$$

The use of these formulas naturally requires the additional storage for Δs_{j-2} .

A projected Δs_j may also be derived with error of order $(\Delta z)^3$ by constructing a Taylor series about $z = z_j$:

$$s = s_j + s'_j(z - z_j) + \frac{1}{2} s''_j(z - z_j)^2 + \frac{1}{6} s'''_j(z - z_j)^3 + \dots$$

and substituting for previously found points:

$$s_{j-1} = s_j - s'_j \Delta z + \frac{1}{2} s''_j \Delta z^2 - \frac{1}{6} s'''_j \Delta z^3 + \dots$$

$$s_{j-2} = s_j - 2s'_j \Delta z + \frac{4}{2} s''_j \Delta z^2 - \frac{8}{6} s'''_j \Delta z^3 + \dots$$

$$s_{j-3} = s_j - 3s'_j \Delta z + \frac{9}{2} s''_j \Delta z^2 - \frac{27}{6} s'''_j \Delta z^3 + \dots$$

By eliminating s'_j and s''_j , we get

$$3s_{j-1} - 3s_{j-2} + s_{j-3} = s_j - s'''_j \Delta z^3 + \dots$$

or

$$\Delta s_j = 2\Delta s_{j-1} - \Delta s_{j-2} + O(\Delta z^3)$$

Appendix C. Program Description and Listing

In the listing of the computer program (presented on pages 30-40), the main program, POLMD2, utilizes the following subroutines to simplify the flow.

FUNCT--Reads in the main data, computes some needed constants and all needed functions of η at half-integer stations by quadratic interpolation.

TERP2N (not listed)--Called by FUNCT to perform quadratic interpolation.

INITLZ--Initializes all variables and computes other needed constants.

The subroutines FUNCT, TERP2N, and INITLZ were overlayed by subsequent subroutines, since they are needed only at the start of the run.

XSTEP--Steps z and computes all constants that are functions of z only.

EMPTY--Initializes the A_i , B_i , and C_i matrices, and the f_i vector to 0. Note that the A_i matrix is called X in the program, the B_i is called BB , and the C_i matrix is adjoined with the f_i vector to form a 5×6 matrix called D . (This permits the later computation of $A_i^{-1}C$ and $A_i^{-1}f_i$ in one operation.)

EMPTY starts the minor i loop, the purpose of which is to eliminate the i -th block of five equations

$$B_i \begin{pmatrix} \Delta s_i^+ \\ \Delta s_i^- \\ \Delta J_i^+ \\ \Delta J_i^- \\ (\Delta \phi_\eta)_j \big|_{i-1} \end{pmatrix} + A_i \begin{pmatrix} \Delta s_j^+ \\ \Delta s_j^- \\ \Delta J_j^+ \\ \Delta J_j^- \\ (\Delta \phi_\eta)_j \big|_i \end{pmatrix} + C_i \begin{pmatrix} \Delta s_j^+ \\ \Delta s_j^- \\ \Delta J_j^+ \\ \Delta J_j^- \\ (\Delta \phi_\eta)_j \big|_{i+1} \end{pmatrix} = f_i$$

($B_i = 0$ for $i = 1$ and $C_i = 0$ for $i = N + 1$) where the subscript j indicates that $z = j\Delta z$.

FIRST, SECOND, THIRD, FOURTH, FIFTH--are entries into EMPTY that fill the X , BB , and D matrices line by line. Note that single subscript arithmetic is used to conserve computer time and core.

ENDO, END1--are called when $i = 1$ and $N + 1$ to take the boundary conditions into account.

BOUND0, BOUND1--define the boundary conditions at $\eta = 0$ and $\eta = 1$. This is the only subroutine the user must write if his boundary conditions differ from equations (16) and (17). [Actually, the supplied BOUND1 contained the condition that $\phi_\eta(x,1) = P_1\delta$; P_1 was read in to be 0 to satisfy equation (17).]

XDCORR--corrects the A_i and f_i arrays by the matrix multiplication:

$$A_i = A_i - B_i \Gamma_{i-1}, \quad i = 2, 3, \dots, N+1$$

$$f_i = f_i - B_i y_{i-1}, \quad i = 2, 3, \dots, N+1$$

as required by the algorithm.³

To speed the process, only the possible nonzero elements of B_i were used and every term was written out.

GELG (not listed)--computes $A_i^{-1}D$ by Gaussian elimination using complete pivoting.

The first five columns of $A_i^{-1}D$ are stored as the Γ_i array (in the computer Z array) and the last column of $A_i^{-1}D$ is stored as the y_i array (in the computer XX array).

REST--does the rest of the computation in the i loop:

1. Back multiplies to find the variables.
2. Updates all needed variable functions of η and some functions of x .
3. Determines if a printout is required for the value of z just completed.
4. If a printout is needed, computes ϕ_j by rectangular formulas, retransforms to $\frac{z}{J}$ from $\frac{z}{J'}$, and computes other functions as needed for the printout. A sample printout is shown in table C-I on page 41.

In the main program, the unlabeled COMMON is placed in equivalence with the Z array to save core. All input data and some variables needed in the FUNCT, INITLZ, and REST routines are not needed during the i loop and can be shared with the Z array. Liberal use of labeled COMMONS served to otherwise transfer data from subroutine to subroutine.

³Isaacson, E. and Keller, H.B., "Analysis of Numerical Methods," John Wiley & Sons, New York, 1966, pp. 58-61.

POLMO2 - - - EFN - SOURCE STATEMENT - - IFN(S) - -

```

DIMENSION Z(10000)
COMMON ETAPT(100),PPT(300),ETALG(100),BOB(200),TPT2(100),DPT(100),
1 O(2),F1(3),PHJ(401),NE2,XN,XZ,XEND,XPRINT,ENE,DY,YO,ETA1,XI,Y,
2 EXPD,UPLS,A1,A2,A3,DELTA,X,JOP,JOM,VSM,PHIY,PSYSP,DSYSM,SNM,
3 TSYSP,TSYSM
COMMON/CONST1/XJ,DELJX,ZJ,D125,DELJ
COMMON/CONST2/P1,P2,P3,P4,P5,P6
COMMON/CONST3/ DELZ,CDEL2,RHOCE,VUX,ENEE,XZ12,XJ12,DELJ12,DELJX2,
1 DZ252,C(8),V,NE,CDEL,CDELE,DELTA,DELTA
COMMON/FUN1/DPLUS(400),DMINUS(400),EP(400),ETA98(400),T29(400),
1 S(400),FPEY(400),KFNO(400),OYCY(400),P(400),T29M(400)
COMMON/FUN2/ B1,B1,KFNO,KFNO1
COMMON/FUN3/ ETAG(51),FQ(51),DTPLQ(51),FPO(51),PO(51),DPLUQ(51),
1 DPHIQ(51),ETA9C(51)
COMMON/INITLZ/PHIJ(401),SPJ(401),SMJ(401),JPJ(401),JMJ(401),
1 USPJ(401),DSMJ(401),SPJH(400),SMJH(400),PHIJH(400)
COMMON/MAT1/X(25),D(30),BB(25)
COMMON/MAT2/XX(2005)
COMMON/INOL/ I,J,M,II,JJ,K
COMMON/INDX/ IDX(6)
COMMON/NUMB/ N,NH,NP1,NC,NCJUNT
EQUIVALENCE (Z(1),ETAPT(1))
REAL JOP,JOM,KFNO,JPJ,JMJ,NE,NE2,KFNO0,KFNO1
C COMPUTE FUNCTIONS
CALL FUNCT
C INITIALIZE ALL VARIABLES
CALL INITLZ
C ROUTINES FUNCT, INITLZ, AND TEPP2N ARE NO LONGER NEEDED.
C MAJOR Z LOOP
DO 999 J = 1,M
C INITIALIZE X FUNCTIONS.
CALL XSTEP
C MINOR ETA LOOP
DO 900 I = 1,NP1
C EMPTY AND FILL X, D, AND BB MATRICES WITH A, C AND F, AND B.
CALL EMPTY
IF(I.EQ.1) GO TO 10
IF(I.EQ.NP1) GO TO 20
CALL FIRST
CALL SECOND
CALL THIRD
CALL FOURTH
CALL FIFTH
GO TO 3
10 CALL ENDO
GO TO 150
20 CALL ENO1
C CORRECT FOR B WHEN I NOT EQUAL TO 1
3 CALL XDCORR(Z)
C READY TO INVERT
150 CALL GELG(D,X,5,6)
C TRANSFER GAMMA MATRICES AND Y VECTOR TO STORAGE.
IF(I.EQ.NP1) GO TO 200
JJ = 25*(I-1)
DO 150 II = 1,25

```

NOT REPRODUCIBLE

```

      X = II + JJ
160 Z(K) = D(II)
200 JJ = 5*(I-1)
      DO 210 II = 1,5
      K = JJ + II
210 XX(K) = D(II+25)
C   END OF ETA LOOP.
900 CONTINUE
C   UPDATE AND WRITE IN REST ROUTINE.
      CALL REST(Z)
C   END OF Z LOOP.
999 CONTINUE
      STOP
      END

```

-----FUNCT.-----EFN-----SOURCE STATEMENT-----IFN(S)-----

```

SUBROUTINE FUNCT
COMMON ETAPT(100),PPT(300),ETALG(100),BOB(200),TPT2(100),DPT(100),
1 Q(2),F1(3),PHJ(401),NE2,XH,XZ,XEND,XPRINT,ENE,DY,YO,ETAI,XI,Y,
2 EXPO,DPLS,A1,A2,A3,DELTA,X,JOP,JOM,VSM,PHIY,DSYSP,DSYSM,SNM,
3 TSYSP,TSYSM
COMMON/CONST3/ DELZ,CDEL2,RHOECE,VOX,ENEE,XZ12,XJ12,DELJ12,DELJX2,
1 DZ252,C(8),V,NE,CDEL,CDELS,DDDELTA,DELTA
COMMON/FUN1/DPLUS(400),UMINUS(400),EP(400),ETA98(400),T29(400),
1 B(400),FPEY(400),KFNO(400),DYEY(400),P(400),T29M(400)
COMMON/FUN2/ B0,B1,KFNO0,KFNO1
COMMON/FUN3/ ETA0(51),FQ(51),DTPLQ(51),FPQ(51),PQ(51),DPLU0(51),
1 DPMIQ(51),ETA30(51)
COMMON/IND1/ I,J,M,II,JJ,K
COMMON/NUMB/ N,NW,NP1,NC,NCOUNT
REAL NE,NE2,JOP,JOM,KFNO,KFNO0,KFNO1
READ(5,1000) V,CDEL,RHOECE,NE,CDEL2
1000 FORMAT(6E13.5)
READ(5,30) II,JJ,K
30 FORMAT(3I5)
READ(5,1000)( ETAPT(I),I=1,II)
READ(5,1000)( PPT(I),I=1,II)
J = II + 1
N = II + II
READ(5,1000)( PPT(I),I=J,N)
J = N + 1
N = N + II
READ(5,1000)( PPT(I),I=J,N)
READ(5,1000)( BOB(I),I=1,JJ)
J = JJ + 1
N = JJ + JJ
READ(5,1000)( BOB(I),I=J,N)
READ(5,1000)( TPT2(I),I=1,K)
READ(5,1000)( DPT(I),I=1,K)
DO 5 I = 1,JJ
ETALG(I) = ALOG(ETAPT(I))
N = JJ + I
BOB(N) = ALOG(BOB(N))
5 BOB(I) = ALOG(BOB(I))
READ(5,1000) XH, XZ,XEND,XPRINT,YO,DY
N = XN
NW = N/50
IF(NW.EQ.0) NW = 1
NE2 = NE*NE*.00375
VSM = DY - YO
DY = VSM/XN
B1 = EXP(YO)
NP1 = N + 1
DO 10 I = 1,N
XI = FLOAT(I) - .5
Y = YO + XI/XN *VSM
EXPO = EXP(Y)
DYEY(I) = 1./EXPO/DY
ETAI = EXPO - B1
B0 = ETAI**.125
ETA98(I) = B0*ETAI

```

NOT REPRODUCIBLE

```

IF(ETAI .GT..0001) GO TO 7
F1(1) = PPT(1)
F1(2) = PPT(11 + 1)
F1(3) = -.8*ETA98(1)
KFNO(1) = BOB(1) + BOB(JJ+1)
GO TO 8
7 CALL TERP2N(11,3,ETAI ,ETAPT,PPT,F1)
XI = ALOG(ETAI )
CALL TERP2N(JJ,2, XI,ETALG,BOB,Q)
KFNO(1) = Q(1) + Q(2)
8 CALL TERP2N( K,1,F1(2),TPT2,DPT,DPLS)
P(1) = F1(1)
T29(1) = 5800./F1(2)*DPLS
EP(1) = BO/P(1)
DPLUS(1) = DPLS*2.
DMINUS(1) = 234.*DPLUS(1)
ETA98(1) = ETA98(1)*CDEL2*2.
T29M(1) = T29(1)*234.
FPEY(1) = F1(3)/P(1)*DYEY(1)
XI = F1(2)**.5
KFNO(1) = EXP(KFNO(1) - 32500./F1(2) - 23.718998)/XI
10 B(1) = NE2/F1(2)/XI /P(1)/P(1)
DO 20 I = 1,51
XI = 1-1
Y = YO + XI/50. *VSM
EXPO = EXP(Y)
ETAQ(1) = EXPO - B1
IF(1.EQ.1) ETAQ(1) = 0.
ETA9Q(1) = ETAQ(1)**1.125
IF(ETAQ(1).GT..0001) GO TO 27
F1(1) = PPT(1)
F1(2) = PPT(11 + 1)
F1(3) = -.8*ETA9Q(1)
GO TO 28
27 CALL TERP2N(11,3,ETAQ(1),ETAPT,PPT,F1)
28 CALL TERP2N( K,1,F1(2),TPT2,DPT,DPLS)
PQ(1) = F1(1)
FQ(1) = F1(3)
FPQ(1) = F1(3)/F1(1)
DPLUQ(1) = DPLS
DPMIQ(1) = DPLS*234.
ETA9Q(1) = ETA9Q(1)*CDEL2
20 DTPLO(1) = 11600./F1(2)*DPLS
I = 11 + 1
XI = PPT(1)**.5
BO = NE2/ PPT(1)/XI/PQ(1)/PQ(1) *4.
KFNOO = BOB(JJ+1) + BOB(1)
KFNOO = EXP(KFNOO - 32500./ PPT(1) - 23.718998)/XI
I = 11 + 11
XI = PPT(1)**.5
B1 = NE2/ PPT(1)/XI/PQ(51)/PQ(51) *4.
CALL TERP2N(JJ,2,0.,ETALG,BOB,Q)
KFNO1 = Q(1) + Q(2)
KFNO1 = EXP(KFNO1 - 32500./ PPT(1) - 23.718998)/XI
RETURN
END

```

INIT. - EFN SOURCE STATEMENT - IFN(S) -

```

SUBROUTINE INITLZ
COMMON ETAPT(100),PPT(300),ETALC(100),BOB(200),TPTZ(100),DPT(100),
1 O(2),F1(3),PHJ(401),NE2,XN,XZ,XEND,XPRINT,ENE,DY,YO,ETAI,XI,Y,
2 EXPO,DPLS,A1,A2,A3,DELTA,X,JOP,JOM,VSM,PHIY,DSYSP,DSYSM,SNM,
3 TSYSP,TSYSM
COMMON/CONST1/XJ,DELJX,ZJ,DZ25,DELJ
COMMON/CONST2/P1,P2,P3,P4,P5,P6
COMMON/CONST3/ DELZ,CDEL2,RHOECB,VDX,ENEE,XZ12,XJ12,DELJ12,DELJX2,
1 DZ252,C(8),V,VE,CDEL,CDELE,DELTA,DELTA
COMMON/INTLZ/PHIJ(401),SPJ(401),SMJ(401),JPJ(401),JMJ(401),
1 DSPJ(401),DSMJ(401),SPJH(400),SMJH(400),PHIJH(400)
COMMON/IND1/ I,J,M,II,JJ,K
COMMON/INDX/ IDX(6)
COMMON/NUM3/ N,NW,NP1,NC,NCOUNT
REAL NE,NE2,JOP,JOM,JPJ,JMJ
READ(5,10) PHIJ(1),P1,P2,P3,P4,P5,P6
10 FORMAT(7E10.5)
READ(5,11) IDX(1),IDX(2),IDX(3),IDX(4),IDX(5),IDX(6)
11 FORMAT(5I5)
XEND = XEND**3
CDEL2 = CDEL*CDEL
ENE = 1.6E-19*VE
ENEE = ENE/8.85E-14*.5
CDELE = CDEL/ENE
DO 21 I = 1,N
PHIJ(I) = PHIJ(I)
PHIJH(I) = PHIJ(I) + PHIJ(I)
SPJH(I) = 0.
SMJH(I) = 0.
SPJ(I) = 0.
SMJ(I) = 0.
JPJ(I) = 0.
JMJ(I) = 0.
DSPJ(I) = 0.
21 DSMJ(I) = 0.
PHIJ(NP1) = PHIJ(1)
SPJ(NP1) = 0.
SMJ(NP1) = 0.
JPJ(NP1) = 0.
JMJ(NP1) = 0.
DSPJ(NP1) = 0.
DSMJ(NP1) = 0.
XJ = 0.
DELJX = 0.
DELJ = 0.
ZJ = 0.
DZ25 = 0.
NC = 0
NCOUNT = XZ/XPRINT
M = XZ
DELZ = XEND/XZ
VDX = .2*V/DELZ
DELTA = CDEL*DELZ
RETURN
END

```

NOT REPRODUCIBLE

----- STEP. ----- EFN SOURCE STATEMENT ----- IFN(S) -----

```

SUBROUTINE XSTEP
COMMON/CONST1/XJ,DELJX,ZJ,DZ25,DELJ
COMMON/CONST3/ DELZ,CDEL2,RHOECE,VDX,ENEE,XZ12,XJ12,DELJ12,DELJX2,
1 DZ252,C(8),V,NE,CDEL,CDELE,DDELTA,DELTA
COMMON/IND1/ I,J,M,II,JJ,K
REAL NE
XZ12 = ZJ + DELZ
DELTA = CDEL*XZ12
DELJ12 = DELTA*DELTA
XJ12 = XZ12**1.25
DELJX2 = DELJ12/XJ12
DZ252 = DELJ12/(XZ12**1.25)
C( 8) = DELJ12 - DELJ
C( 1) = DELJ12/RHOECE
C( 2) = VDX*(3.*DZ252 - DZ25)
IF(J.EQ.1) C(2) = C(2)/.75
C( 3) = V *DELJX2
C( 4) = ENEE*DELJ12
C( 5) = V *(DELJX2 - DELJX)
C( 6) = C( 8)/RHOECE
C( 7) = VDX*(DZ252 + DZ25)
C( 8) = ENEE*C( 8)
RETURN
END

```

----- BOUND. ----- EFN SOURCE STATEMENT ----- IFN(S) -----

```

SUBROUTINE BOUND0
COMMON/FUN3/ ETAQ(51),FQ(51),DTPLQ(51),FPQ(51),PQ(51),DPLUQ(51),
1 DPMI(51),ETA9Q(51)
COMMON/INTLZ/PHIJ(401),SPJ(401),SMJ(401),JPJ(401),JMJ(401),
1 DSPJ(401),DSMJ(401),SPJH(400),SMJH(400),PHIJH(400)
COMMON/MAT1/X(25),D(30),RB(25)
COMMON/CONST3/ DELZ,CDEL2,RHOECE,VDX,ENEE,XZ12,XJ12,DELJ12,DELJX2,
1 DZ252,C(8),V,NE,CDEL,CDELE,DDELTA,DELTA
COMMON/CONST2/P1,P2,P3,P4,P5,P6
COMMON/CONST1/XJ,DELJX,ZJ,DZ25,DELJ
REAL JPJ,JMJ,NE
X(3) = 10.E10
X(9) = 10.E10
D(28) = 0.
D(29) = 0.
RETURN
ENTRY BOUND1
X( 1) = 10.E10
X( 7) = 10.E10
X(25) = 10.E10
D(26) = 0.
D(27) = 0.
D(30) = P1*DDELTA*X(1)
RETURN
END

```

EMPTY. - EFN SOURCE STATEMENT - IFN(S) -

```

SUBROUTINE EMPTY
COMMON/CONST3/ DELZ,CDEL2,RHOECE,VDX,ENEE,XI12,XJ12,DELJ12,DELJX2,
1 DZ252,C(8),V,NE,CDEL,CDELE,ODELTA,DELTA
COMMON/FUN1/DPLUS(400),DMINUS(400),EP(400),ETA98(400),T29(400),
1 B(400),FPEY(400),KFNO(400),DYEY(400),P(400),T29H(400)
COMMON/INTLZ/PHIJ(401),SPJ(401),SMJ(401),JPJ(401),JMJ(401),
1 DSPJ(401),DSMJ(401),SPJH(400),SMJH(400),PHIJH(400)
COMMON/MAT1/X(25),D(30),BB(25)
COMMON/IND1/ I,J,M,II,JJ,K
COMMON/INDX/ IDX(6)
REAL NE, JPJ,JMJ,KFNO
DD SC 11 = 1.25
BB(11) = 0.
X(11) = 0.
50 D(11) = 0.
RETURN
ENTRY FIRST
K = 1-IDX(1)
D(25) = DDELTA*ETA98(K)
X(11) = DPLUS(K) + DELTA*ETA98(K)
D(26) = D(26)/(X(11) - D(26))
X(11) = T29(K)/X(11)
X(21) = X(1)*(SPJH(K) + DSPJ(K+1) + DSPJ(K))
X(1) = X(1)*PHIJH(K)
X(11) = -P(K)/X(11)
D(26) = (X(1)*SPJH(K) + X(11)*(JPJ(K+1)+JPJ(K)))*D(26)
IF(IDX(1).EQ.1) GO TO 80
D(1) = X(1) + DYEY(K)
X(1) = X(1) - DYEY(K)
D(11) = X(11)
D(21) = X(21)
RETURN
80 BB(1) = X(1) - DYEY(K)
X(1) = X(1) + DYEY(K)
BB(11) = X(11)
BB(21) = X(21)
RETURN
ENTRY SECDND
K = 1 - IDX(2)
D(27) = DDELTA*ETA98(K)
X(17) = DMINUS(K) + DELTA*ETA98(K)
D(27) = D(27)/(X(17)-D(27))
X(7) = -T29H(K)/X(17)
X(22) = X(7)*(SMJH(K) + DSMJ(K+1) + DSMJ(K))
X(7) = X(7)*PHIJH(K)
X(17) = -P(K)/X(17)
D(27) = (X(7)*SMJH(K) + X(17)*(JMJ(K+1)+JMJ(K)))*D(27)
IF(IDX(2).EQ.1) GO TO 10
D(7) = X(7) + DYEY(K)
X(7) = X(7) - DYEY(K)
D(17) = X(17)
D(22) = X(22)
RETURN
10 BB(7) = X(7) - DYEY(K)
X(7) = X(7) + DYEY(K)

```

```

      BB(17) = X(17)
      BB(22) = X(22)
      RETURN
      ENTRY THIRD
      K = I - I0X(3)
      X(1) = B(K)*C(1)
      X(3) = -X(8)*SMJH(K) - C(2)*EP(K)
      X(13) = -X(9)*(SPJH(K) + DSPJ(K+1) + DSPJ(K))
      X(13) = C(3)*FPEY(K)
      D(25) = C(5)*FPEY(K)*(SPJ(K+1) - SPJ(K)) + C(6)*(-KFND(K) + B(K)*
1 SPJH(K)*SMJH(K)) - C(7)*EP(K)*(DSPJ(K+1) + DSPJ(K))
      IF(I0X(3).EQ.1) GO TO 20
      D(1) = X(3) - X(13)
      X(3) = X(3) + X(13)
      D(8) = X(1)
      D(13) = DYEY(K)
      X(13) = -DYEY(K)
      RETURN
20 BB(3) = X(3) + X(13)
      X(3) = X(3) - X(13)
      BB(8) = X(8)
      BB(13) = -DYEY(K)
      X(13) = DYEY(K)
      RETURN
      ENTRY FOURTH
      K = I - I0X(4)
      X(4) = B(K)*C(1)
      X(9) = -X(4)*SPJH(K) - C(2)*EP(K)
      X(4) = -X(4)*(SMJH(K) + DSMJ(K+1) + DSMJ(K))
      X(13) = C(3)*FPEY(K)
      D(29) = C(5)*FPEY(K)*(SMJ(K+1) - SMJ(K)) + C(6)*(-KFND(K) + B(K)*
1 SPJH(K)*SMJH(K)) - C(7)*EP(K)*(DSMJ(K+1) + DSMJ(K))
      IF(I0X(4).EQ.1) GO TO 30
      D(4) = X(4)
      D(9) = X(9) - X(19)
      X(9) = X(9) + X(19)
      D(19) = DYEY(K)
      X(19) = -DYEY(K)
      RETURN
30 BB(4) = X(4)
      DD(9) = X(9) + X(19)
      X(9) = X(9) - X(19)
      BB(19) = -DYEY(K)
      X(19) = DYEY(K)
      RETURN
      ENTRY FIFTH
      K = I - I0X(5)
      X(5) = C(4)/P(K)
      X(10) = -X(5)
      C(30) = -C(8)/P(K)*(SPJH(K)-SMJH(K))
      IF(I0X(5).EQ.1) GO TO 40
      D(5) = X(5)
      D(10) = X(10)
      D(25) = DYEY(K)
      X(25) = -DYEY(K)
      RETURN
40 BB(5) = X(5)
      BB(10) = X(10)
      DD(25) = -DYEY(K)
      X(25) = DYEY(K)
100 RETURN
      END

```

```

----- REST. ----- EFN SOURCE STATEMENT ----- IFN(S) -----

SUBROUTINE REST(Z)
  DIMENSION Z(10000)
  COMMON ETAPT(100),PPT(300),ETALG(100),BOB(200),TPT2(100),DPT(100),
1 Q(2),F1(3),PHJ(401),NE2,XN,XZ,XEND,XPRINT,ENE,DY,YO,ETA1,XI,Y,
2 EXPO,DPLS,A1,A2,A3,DELTA,X,JOP,JOM,VSM,PHIY,DSYSP,DSYSM,SNM,
3 TSYSP,TSYSM
  COMMON/CONST1/XJ,DELJX,ZJ,DZ25,DELJ
  COMMON/CONST2/P1,P2,P3,P4,P5,P6
  COMMON/CONST3/ DELZ,CDEL2,RHOECE,VDX,ENEE,XZ12,XJ12,DELJ12,DELJX2,
1 DZ252,C(8),V,NE,CDEL,CDELE,DDELTA,DELTA
  COMMON/FUN1/DPLUS(400),DMINUS(400),EP(400),ETA98(400),T29(400),
1 B(400),FPEY(400),KFNO(400),DYEY(400),P(400),T29M(400)
  COMMON/FUN3/ ETAQ(51),FO(51),DTPLQ(51),FPO(51),PQ(51),DPLUQ(51),
1 DPMIQ(51),ETA9C(51)
  COMMON/INTLZ/PHIJ(401),SPJ(401),SMJ(401),JPJ(401),JMJ(401),
1 DSPJ(401),DSMJ(401),SPJH(400),SMJH(400),PHIJH(400)
  COMMON/MAT2/XX(2005)
  COMMON/IND1/ I,J,M,II,JJ,K
  COMMON/INDX/ IDX(6)
  COMMON/NUMB/ N,NW,NP1,NC,NCOUNT
  REAL JOP,JOM,KFNO,JPJ,JMJ,NE,NE2
C   READY FOR BACK MULTIPLICATION
  JJ = 5*N
  II = 25*N
  DO 250 I = 1,N
    II = II - 25
    JJ5 = JJ
    JJ = JJ-5
    DO 250 K = 1,5
      L1 = JJ + K
      L2 = II + K
      DO 250 L = 1,5
        L3 = JJ5 + L
        XX(L1) = XX(L1) - Z(L2)*XX(L3)
      250 L2 = L2 + 5
    C   ANSWERS ARE IN XX ARRAY. WRITE AND UPDATE BEFORE STEPPING X.
    K = -4
    DO 260 I = 1,NP1
      K = K + 5
      DSPJ(I) = XX(K)
      DSMJ(I) = XX(K+1)
      SPJ(I) = SPJ(I) + DSPJ(I)
      SMJ(I) = SMJ(I) + DSMJ(I)
      JPJ(I) = JPJ(I) + XX(K+2)
      JMJ(I) = JMJ(I) + XX(K+3)
      PHIJ(I) = PHIJ(I) + XX(K+4)
      IF(I.EQ.1) GO TO 260
      II = I-1
      SPJH(II) = SPJ(I) + SPJ(II)
      SMJH(II) = SMJ(I) + SMJ(II)
      PHIJH(II) = PHIJ(I) + PHIJ(II)
    260 CONTINUE
    XJ = XJ12
    DELJ = DELJ12
    DELJX = DELJX2

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NOT REPRODUCIBLE

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ZJ = XZ12
DZ25 = DZ252
NC = NC + 1
IF (NC.LT.NCOUNT) RETURN
NC = 0
C WRITE HEADING
WRITE(5,1001) XJ,DELZ,N
1001 FORMAT(5H1X = ,F7.2,5X,10HDELTA Z. = ,F9.4,5X,16HETA-INTERVALS = ,
113,/80X,5HKPLUS,4X,6HD PLUS,9H D MINUS,3X,6HDTPLUS,9H DTMINUS /
23X,5HETA,5X,6HMINUS,4X,5HSPPLUS,4X,6HSMINUS,5X,5HJPLUS,4X,6HJMINUS
3,4X,5HPHIETA,5X,3HPHI,7X,2H-V,5X,5H*PHIY,4X,5H*SY/S,4X,5H*SY/S,
44X,5H*SY/S,4X,5H*SY/S //)
C COMPUTE PHI ( = PHJ)
IF (IDX(5).EQ.1) GO TO 251
PHJ(NP1) = 0.
DO 252 I = 1,N
K = NP1 - I
252 PHJ(K) = PHJ(K+1) - .5*PHIJH(X)/DYEY(K)
GO TO 275
251 PHJ(1) = 0.
DO 253 I = 1,N
253 PHJ(I+1) = PHJ(I) + .5*PHIJH(I)/DYEY(I)
275 A1 = V*DELJX
A2 = COELE*ZJ
DELTAX = -DELTA/XJ*V
I1 = 0
DO 300 I = 1,NP1,NW
I1 = I1 + 1
A3 = A1*FPO(I1)
JOP = (JPJ(I1) - A3*SPJ(I1))/A2
JOM = (JMJ(I1) - A3*SMJ(I1))/A2
A3 = PQ(I1)/DELTA
VSM = DELTAX*FQ(I1)
SNM = NE*SN1(I1)/PO(I1)
PHIY = DTPLU(I1)*PHIJ(I1)/DELTA
DSYSP = -PHIY + A3*JPJ(I1)/SPJ(I1)
DSYSM = PHIY*234. + A3*JMJ(I1)/SMJ(I1)
A3 = ETA9Q(I1)*DELTA
TSYSP = DPLUC(I1) + A3
TSYSM = DPMIC(I1) + A3
DSYSP = DSYSP*DPLUQ(I1)/TSYSP
DSYSM = DSYSM*DPMIO(I1)/TSYSM
TSYSP = DSYSP*A3/DPLUQ(I1)
TSYSM = DSYSM*A3/DPMIO(I1)
IF (SPJ(I1).NE.0.) GO TO 280
DSYSP = 1.E38
TSYSP = 1.E38
280 IF (SMJ(I1).NE.0.) GO TO 300
DSYSM = 1.E38
TSYSM = 1.E38
300 WRITE(5,1003) ETAG(I1),SNM,SPJ(I1),SMJ(I1),JOP,JOM,PHIJ(I1),PHJ(I1),
1 VSM,PHIY,DSYSP,DSYSM,TSYSP,TSYSM
1003 FORMAT(1P2E9.2,1P5E10.3,1P7E9.2)
IF (XJ.GT.P6) STOP
RETURN
END

```

----- XDCOR. ----- EFN SOURCE STATEMENT ----- IFN(S) -----

```

SUBROUTINE XDCORR(Z)
  DIMENSION Z(10000)
  COMMON/MAT1/X(25),D(30),JB(25)
  COMMON/MAT2/XX(2005)
  COMMON/IND1/ I,J,K,II,JJ,K
  COMMON/INDX/ IDX(6)
  JJ = 25*(I-2)
  JJ0 = 5*I - 9
  JJ1 = JJ0 + 1
  JJ2 = JJ0 + 2
  JJ3 = JJ0 + 3
  JJ4 = JJ0 + 4
  IF(IDX(1).EQ.0) GO TO 7
  DO 5 II = 1,21,5
    K = JJ + II
    5 X(II) = X(II)-BB(1)*Z(K)-BB(11)*Z(K+2)-BB(21)*Z(K+4)
    D(25)=D(25)-BB(1)*XX(JJ0)-BB(11)*XX(JJ2)-BB(21)*XX(JJ4)
    7 IF(IDX(2).EQ.0) GO TO 12
    DO 10 II = 2,22,5
      K = JJ + II
      10 X(II) = X(II)-BB(7)*Z(K)-BB(17)*Z(K+2)-BB(22)*Z(K+3)
      D(27)=D(27)-BB(7)*XX(JJ1)-BB(17)*XX(JJ3)-BB(22)*XX(JJ4)
      12 IF(IDX(3).EQ.0) GO TO 17
      DO 15 II = 3,23,5
        K = JJ + II
        15 X(II) = X(II)-BB(3)*Z(K-2)-BB( 8)*Z(K-1)-BB(13)*Z(K)
        D(28)=D(28)-BB(3)*XX(JJ0)-BB( 8)*XX(JJ1)-BB(13)*XX(JJ2)
      17 IF(IDX(4).EQ.0) GO TO 22
      DO 20 II = 4,24,5
        K = JJ + II
        20 X(II) = X(II)-BB(4)*Z(K-3)-BB( 9)*Z(K-2)-BB(19)*Z(K)
        D(29)=D(29)-BB(4)*XX(JJ0)-BB( 9)*XX(JJ1)-BB(19)*XX(JJ3)
      22 IF(IDX(5).EQ.0) RETURN
      DO 25 II = 5,25,5
        K = JJ + II
        25 X(II) = X(II)-BB(5)*Z(K-4)-BB(10)*Z(K-3)-BB(25)*Z(K)
        D(30)=D(30)-BB(5)*XX(JJ0)-BB(10)*XX(JJ1)-BB(25)*XX(JJ4)
      RETURN
    END

```

----- ENDO. ----- EFN SOURCE STATEMENT ----- IFN(S) -----

```

SUBROUTINE ENDO
  COMMON/INDX/ IDX(6)
  IF(IDX(1).EQ.0) CALL FIRST
  IF(IDX(2).EQ.0) CALL SECOND
  IF(IDX(3).EQ.0) CALL THIRD
  IF(IDX(4).EQ.0) CALL FOURTH
  IF(IDX(5).EQ.0) CALL FIFTH
  CALL BOUND0
  RETURN
  ENTRY ENDO
  IF(IDX(1).EQ.1) CALL FIRST
  IF(IDX(2).EQ.1) CALL SECOND
  IF(IDX(3).EQ.1) CALL THIRD
  IF(IDX(4).EQ.1) CALL FOURTH
  IF(IDX(5).EQ.1) CALL FIFTH
  CALL BOUND1
  RETURN
  END

```


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